

Two charges on plane in a magnetic field: II. Moving neutral quantum system across a magnetic field

M.A. Escobar-Ruiz* and A.V. Turbiner†

*Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México,
Apartado Postal 70-543, 04510 México, D.F., Mexico*

(ΩDated: June 27, 2014)

Abstract

The moving neutral system of two Coulomb charges on a plane subject to a constant magnetic field B perpendicular to the plane is considered. It is shown that the composite system of finite total mass is bound for any center-of-mass momentum P and magnetic field strength; the energy of the ground state is calculated accurately using a variational approach. Their accuracy is cross-checked in a Lagrange-mesh method for $B = 1$ a.u. and in a perturbation theory at small B and P . The constructed trial function has the property of being a uniform approximation of the exact eigenfunction. For a Hydrogen atom and a Positronium a double perturbation theory in B and P is developed and the first corrections are found algebraically. A phenomenon of a sharp change of energy behavior for a certain center-of-mass momentum and a fixed magnetic field is indicated.

*Electronic address: mauricio.escobar@nucleares.unam.mx

†Electronic address: turbiner@nucleares.unam.mx

Introduction

Two-dimensional planar systems of several Coulomb charges of finite masses, both classical and quantum, exhibit many interesting properties which are usually either hidden or absent in three dimensional one. The situation gets even more interesting if a magnetic field perpendicular to the plane is imposed. The first non-trivial case of two Coulomb charges reveals the existence of unexpected concentric classical trajectories and straight line motion (for neutral systems) (see [1] and references therein) in classical problem. In the quantum case there exist a certain eigenstates which are characterized by extra quantum numbers. They are the eigenfunctions of the operators which are not global integrals [2]. Usually, these eigenfunctions are of polynomial form (up to a multiplicative factor) [2–4]. In two important cases of quasi-equal charges ($\frac{e_1}{m_1} = \frac{e_2}{m_2}$) and neutral system at rest the hidden algebra $sl(2)$ in finite-dimensional representation is present for a certain discrete values of a magnetic field strength [2, 5]. It is needless to say that in the three-dimensional case there exists the phenomenon of dissociation which is absent in the two-dimensional planar case. All that indicates the absence of a trivial connection between two- and three-dimensional cases. However, it turns out that there exists a number of properties which are similar for two- and three-dimensional systems in a constant uniform magnetic field. This similarity will be mentioned in our presentation.

In our previous paper [6] an accurate variational solution for several low-lying states for both quasi-equal charges ($\frac{e_1}{m_1} = \frac{e_2}{m_2}$) and neutral system at rest was given. The stability of the system was shown for all magnetic fields. The accuracy of the obtained results was evaluated in a specially designed, convergent perturbation theory. The goal of the present paper is to perform the study of the ground state of a moving neutral system of two Coulomb charges of finite masses in a wide range of magnetic fields and to check its stability. It has to be emphasized that the global integral of the motion, the Pseudomomentum \mathbf{K} established by Gor'kov & Dzyaloshinskii [7] for the three-dimensional case remains the global integral for planar case as well, it coincides with the center-of-mass (CMS) canonical momentum of the system, $\mathbf{P} = \mathbf{K}$. We focus on a particular case of the Hydrogen atom (the case of unequal masses) and we also mention Positronium (the case of equal masses). To the best knowledge of the present authors there was a single attempt so far to study the moving Hydrogen atom on the plane carried out by Lozovik *et al*, [8]. It was done for very weak

magnetic fields. This problem is seen as an important for solid state physics, for the physics of excitons.

As a first step we consider the case of weak magnetic fields and small CMS momentum in double perturbation theory in powers of B and P . It will be realized in the "nonlinearization procedure" [9], in the framework of which the computation of the coefficients of the perturbation series is a purely algebraic problem. In the case of larger fields and CMS momenta we are going to employ the variational formalism constructing the trial function in such a way to combine into an interpolation a WKB expansion at large distances with perturbation theory expansion at small distances near the extremum of the potential [11].

I. GENERALITIES

The Hamiltonian, which describes a two-body neutral system, $(e, m_1), (-e, m_2)$ assuming $e > 0$, in a constant and uniform magnetic field B perpendicular to the plane, has of the form,

$$\hat{H} = \frac{(\hat{\mathbf{p}}_1 - e \mathbf{A}_1)^2}{2m_1} + \frac{(\hat{\mathbf{p}}_2 + e \mathbf{A}_2)^2}{2m_2} - \frac{e^2}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|}, \quad \boldsymbol{\rho}_{1,2} \in \mathbb{R}^2, \quad (1)$$

where $\hbar = c = \frac{1}{4\pi\epsilon_0} = 1$, $\hat{\mathbf{p}}_{1,2} = -i \nabla_{1,2}$ is the momentum and $\boldsymbol{\rho}_{1,2}$ is the position vector of the first (second) particle. Here the symmetric gauge $\mathbf{A}_{1,2} = \frac{1}{2} \mathbf{B} \times \boldsymbol{\rho}_{1,2}$ is chosen. It is easy to check that the total Pseudomomentum,

$$\hat{\mathbf{K}} = \hat{\mathbf{p}}_1 + e \mathbf{A}_1 + \hat{\mathbf{p}}_2 - e \mathbf{A}_2, \quad (2)$$

is a vector integral of motion belonging the plane, on where the dynamics is developed,

$$[\hat{H}, \hat{\mathbf{K}}] = 0,$$

as well as the total angular momentum

$$\hat{\mathbf{L}} = \boldsymbol{\rho}_1 \times \hat{\mathbf{p}}_1 + \boldsymbol{\rho}_2 \times \hat{\mathbf{p}}_2, \quad (3)$$

$[\hat{\mathbf{L}}, \hat{H}] = 0$. The vector $\hat{\mathbf{L}}$ is perpendicular to the plane. In general, the problem is not completely integrable.

It is convenient to introduce center-of-mass (c.m.s.) coordinates

$$\begin{aligned} \mathbf{R} &= \mu_1 \boldsymbol{\rho}_1 + \mu_2 \boldsymbol{\rho}_2, & \boldsymbol{\rho} &= \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2, \\ \hat{\mathbf{P}} &= \hat{\mathbf{p}}_1 + \hat{\mathbf{p}}_2, & \hat{\mathbf{p}} &= \mu_2 \hat{\mathbf{p}}_1 - \mu_1 \hat{\mathbf{p}}_2, \end{aligned} \quad (4)$$

where $M = m_1 + m_2$ is the total mass of the system and $\mu_i = \frac{m_i}{M}$ is relative mass of the i th charge. In these coordinates

$$\hat{\mathbf{K}} = \hat{\mathbf{P}} + e \mathbf{A}_\rho , \quad (5)$$

$$\hat{\mathbf{L}} = (\mathbf{R} \times \hat{\mathbf{P}}) + (\boldsymbol{\rho} \times \hat{\mathbf{p}}) \equiv \hat{\mathcal{L}} + \hat{\boldsymbol{\ell}} , \quad (6)$$

(cf. (2), (3)), where $\mathbf{A}_\rho = \frac{1}{2} \mathbf{B} \times \boldsymbol{\rho}$.

It is easy to check that the integrals $\hat{\mathbf{K}} = (\hat{K}_x, \hat{K}_y)$, $\hat{\mathbf{L}} = \hat{L} \mathbf{n}_z$ obey the commutation relations

$$\begin{aligned} [\hat{K}_x, \hat{K}_y] &= 0 , \\ [\hat{L}, \hat{K}_x] &= \hat{K}_y , \\ [\hat{L}, \hat{K}_y] &= -\hat{K}_x , \end{aligned} \quad (7)$$

hence, they span a noncommutative algebra with the Casimir operator $\hat{\mathcal{C}}$,

$$\hat{\mathcal{C}} = \hat{K}_x^2 + \hat{K}_y^2 . \quad (8)$$

It is convenient to make unitary transformation of the canonical momenta

$$U^{-1} \hat{\mathbf{P}} U = \hat{\mathbf{P}} - e \mathbf{A}_\rho , \quad U^{-1} \hat{\mathbf{p}} U = \hat{\mathbf{p}} + e \mathbf{A}_\mathbf{R} ,$$

with

$$U = e^{-ie \mathbf{A}_\rho \cdot \mathbf{R}} . \quad (9)$$

Then, the unitary transformed Pseudomomentum reads

$$\mathbf{K}' = U^{-1} \hat{\mathbf{K}} U = \hat{\mathbf{P}} , \quad (10)$$

it coincides with the c.m.s. momentum of the whole, composite system, see (2). The unitary transformed Hamiltonian (1) takes the form

$$\hat{\mathcal{H}}' = U^{-1} \hat{\mathcal{H}} U = \frac{(\hat{\mathbf{P}} - e \mathbf{B} \times \boldsymbol{\rho})^2}{2M} + \frac{(\hat{\mathbf{p}} - q_w \mathbf{A}_\rho)^2}{2m_r} - \frac{e^2}{\rho} , \quad (11)$$

here $q_w = e(\mu_2^2 - \mu_1^2) = e(\mu_2 - \mu_1)$ is an effective charge (weighted total charge). It is evident, $[\hat{\mathbf{K}}', \hat{\mathcal{H}}'] = 0$. The eigenfunctions of $\hat{\mathcal{H}}'$ and $\hat{\mathcal{H}}$ are related

$$\Psi' = \Psi e^{ie \mathbf{A}_\rho \cdot \mathbf{R}} . \quad (12)$$

It is easy to check that the eigenfunction of $\hat{\mathbf{P}}$ has the form

$$\Psi'_\mathbf{P}(\mathbf{R}, \boldsymbol{\rho}) = e^{i\mathbf{P} \cdot \mathbf{R}} \psi_\mathbf{P}(\boldsymbol{\rho}) , \quad (13)$$

where \mathbf{P} is the eigenvalue and $\psi_{\mathbf{P}}(\boldsymbol{\rho})$ depends on the relative coordinate $\boldsymbol{\rho}$. Substituting $\Psi'_{\mathbf{P}}$ into the Schrödinger equation for $\hat{\mathcal{H}}'$ we obtain the equation of the relative motion

$$h \psi_{\mathbf{P}}(\boldsymbol{\rho}) \equiv \left[\frac{(\hat{\mathbf{p}} - e(\mu_2 - \mu_1) \mathbf{A}_{\boldsymbol{\rho}})^2}{2m_r} + \frac{(\mathbf{P} - e \mathbf{B} \times \boldsymbol{\rho})^2}{2M} - \frac{e^2}{\rho} \right] \psi_{\mathbf{P}}(\boldsymbol{\rho}) = E \psi_{\mathbf{P}}(\boldsymbol{\rho}), \quad (14)$$

where CMS momentum \mathbf{P} plays a role of external parameter.

The equation (14) is the basic equation we are going to study. At $\mathbf{P} = \mathbf{0}$, the relative angular momentum $\hat{\ell}_z = -i \partial_{\varphi}$ is conserved, the relative polar angle φ is separated out and the problem (14) is reduced to a study of dynamics in (relative) radial direction ρ , thus, becomes effectively one-dimensional(!). In double polar coordinates CMS (R, ϕ) and relative (ρ, φ) coordinate systems (i) the eigenfunctions are factorizable, all factors except for ρ -dependent are found analytically, they have definite relative angular momentum, (ii) dynamics in ρ -direction is described by a funnel-type potential and it is characterized by the hidden $sl(2)$ algebra; (iii) at some discrete values of dimensionless magnetic fields $b \equiv \frac{B}{4m_r^2 e^3 c} \leq 1$ the algebra $sl(2)$ emerges in finite-dimensional representation, thus, the system becomes *quasi-exactly-solvable*. This case has been analyzed in [2] (see also [4]).

However, for the case of moving system $\mathbf{P} \neq 0$, an immediate observation is that the relative angular momentum $\hat{\ell}_z$ is not conserved. Consequently, the relative coordinates are not separated and the system is not reduced to one-dimensional dynamics. Neither factorization of eigenfunctions nor a hidden algebraic structure occurs. The problem is essentially two-dimensional and we arrive at the question how to solve it. A simple idea that we are going to employ is to combine a WKB expansion at large distances with perturbation theory near the minima of the potential into an interpolation. The main practical goal of this paper is to construct such an approximation for the ground state of the Hydrogen atom and then use it as variational trial function.

II. ATOM AT SMALL MAGNETIC FIELDS AND SMALL PSEUDOMOMENTUM

Let us first consider the case of weak magnetic fields and small Pseudomomentum. In this regime the interaction of particles with the magnetic field as well as magnetic field self-interaction can be treated as a perturbation of the Hydrogen atom. We focus our analysis

on the ground state only. The wave function depending on relative coordinate $\boldsymbol{\rho}$ (see (13)) can be represented in the form:

$$\psi = e^{-\Phi(\rho, \varphi)} . \quad (15)$$

We assume that the phase $\Phi(\rho, \varphi)$ has no singularities on the real plane. Substituting (15) with CM momentum chosen to be directed along y -axis, thus, $\mathbf{P} = (P, \frac{\pi}{2})$ in polar coordinates, into the Schrödinger equation (14) we arrive at the Riccati type equation

$$\frac{1}{2m_r} \Delta \Phi - \frac{i e B |\mu_2 - \mu_1|}{2m_r} \frac{\partial \Phi}{\partial \varphi} - \frac{1}{2m_r} (\nabla \Phi)^2 = \hat{E} - V , \quad (16)$$

with a non-trivial potential

$$V = \frac{e^2 B^2 \rho^2}{8m_r} - \frac{e B P \rho \cos \varphi}{M} - \frac{e^2}{\rho} , \quad (17)$$

where $\hat{E} = E - \frac{P^2}{2M}$. Now we develop a perturbation theory for Φ and \hat{E}

$$\begin{aligned} \Phi &= \sum_{n,k=0}^{\infty} B^n P^k \Phi_{n,k} , \\ \hat{E} &= \sum_{n,k=0}^{\infty} B^n P^k \hat{E}_{n,k} . \end{aligned} \quad (18)$$

Substituting (18) into (16), and collecting the terms of the order of $B^n P^k$, we obtain the following equation for corrections, thus, $n + k > 0$:

$$\frac{1}{2m_r} \Delta \Phi_{n,k} - \frac{i e B |\mu_2 - \mu_1|}{2m_r} \frac{\partial}{\partial \varphi} \Phi_{n-1,k} - \frac{1}{m_r} \nabla \Phi_{0,0} \nabla \Phi_{n,k} = \hat{E}_{n,k} - Q_{n,k} , \quad (19)$$

where formally $\Phi_{-1,k} = 0$, here $Q_{n,k}$ plays the role of an effective perturbation potential and is given by the following formulas:

$$Q_{0,1} = Q_{1,0} = Q_{0,2} = 0 , \quad Q_{1,1} = -\frac{e \rho \cos \varphi}{M} , \quad Q_{2,0} = \frac{e^2 \rho^2}{8m_r} ,$$

and for $n + k > 2$

$$Q_{n,k} = -\frac{1}{2m_r} \sum_{0 \leq m \leq n, 0 \leq p \leq k} \nabla \Phi_{m,p} \nabla \Phi_{n-m,k-p} , \quad (20)$$

where the summation is performed such a way that $m + p \neq 0$ and $m + p < n + k$. The first corrections in (18) can be calculated explicitly (see Table I for some concrete cases) and the

energy expansion has a form

$$\begin{aligned}
\hat{E} = & -2m_r + \frac{3}{64m_r^3} B^2 - \frac{21}{256m_r^3 M^2} B^2 P^2 - \frac{159(4m_r + M\mu^2)^2}{65536m_r^7 M^2} B^4 \\
& + \frac{3(115M\mu^2 - 2062m_r)}{131072m_r^7 M^3} B^4 P^2 + \frac{17877}{1048576m_r^7 M^4} B^4 P^4 \\
& - \frac{1293475M^2\mu^4 + 1624212m_r M\mu^2 - 1816848m_r^2}{805306368m_r^{11} M^4} B^6 P^2 + \dots
\end{aligned} \tag{21}$$

where we put $e = 1$ and $\mu = \mu_1 - \mu_2$. The coefficient functions in the phase expansion (18)

are

$$\begin{aligned}
\Phi_{0,0} &= 2m_r \rho, \quad \Phi_{1,1} = -\frac{(3 + 4m_r \rho) \rho \sin \varphi}{16m_r M}, \\
\Phi_{2,1} &= -\frac{i\mu(51 + 4m_r \rho(17 + 8m_r \rho)) \rho \cos \varphi}{1536m_r^3 M}, \quad \Phi_{2,0} = \frac{\rho^2(4m_r + M\mu^2)(9 + 8m_r \rho)}{384m_r^2 M}, \\
\Phi_{0,2} &= \frac{\rho^2(-99 - 40m_r \rho + 3(11 + 8m_r \rho) \cos 2\varphi)}{3072m_r^2 M^2}.
\end{aligned} \tag{22}$$

Since in the potential (17) the magnetic field B appears as a coefficients in front of the most singular term $\sim \rho^2$ at large distances the Dyson instability phenomenon occurs when B^2 is negative (for discussion, see [9]). Hence, it is evident that this perturbation theory in powers of B is divergent, there exists a singularity at $B = 0$. Otherwise, for any fixed $B \neq 0$ the Dyson instability phenomenon does not occur when P changes sign. It indicates that the series in P has a finite radius of convergence, which is, of course, of the order of B . Thus, a domain of applicability is limited to the case of fairly low B and $P \lesssim B$.

III. MOVING ATOM IN A ARBITRARY MAGNETIC FIELD AND PSEUDO-MOMENTUM

In this section we consider the neutral system in a magnetic field for arbitrary values of a magnetic field and Pseudomomentum.

\hat{E} (Hartrees)	H ($M < \infty$)	H ($M \rightarrow \infty$)	Ps ($M = 2 a.u.$)
$\hat{E}_{0,0}$	-1.9989	-2	-1
$\hat{E}_{2,0}$	0.04695	$\frac{3}{64}$	$\frac{3}{8}$
$\hat{E}_{4,0}$	-0.002435	$-\frac{159}{65536}$	$-\frac{159}{512}$
$\hat{E}_{2,2}$	-2.4344×10^{-8}	0	$-\frac{21}{128}$
$\hat{E}_{4,2}$	0.7735×10^{-9}	0	$-\frac{3093}{8192}$
$\hat{E}_{4,4}$	1.502×10^{-15}	0	$\frac{17877}{131072}$

Table I: Coefficients $\hat{E}_{i,j}$ in (18) for the Hydrogen atom and Positronium, M is total mass of the system.

A. Scaling relations

One can relate two different neutral systems, (e, m_1, m_2) and $(\tilde{e}, \tilde{m}_1, \tilde{m}_2)$. In order to do it let us make a scale transformation $\rho \rightarrow a \rho$ in (14) and choose

$$a = \frac{\tilde{e}^2 \tilde{m}_r}{e^2 m_r},$$

together with

$$\begin{aligned} \frac{\tilde{B}}{\tilde{e}^3 \tilde{m}_r^2} &= \frac{B}{e^3 m_r^2} \\ \frac{\tilde{P}}{(\tilde{m}_1 + \tilde{m}_2) \tilde{e}^2} &= \frac{P}{(m_1 + m_2) e^2} \\ |\tilde{\mu}_2 - \tilde{\mu}_1| &= |\mu_2 - \mu_1|. \end{aligned}$$

Then the following scaling relations emerge

$$\begin{aligned} \psi_{\mathbf{P}}(\tilde{e}, \tilde{m}_1, \tilde{m}_2, \tilde{B}, \tilde{P}; a\rho, \varphi) &= \psi_{\mathbf{P}}(e, m_1, m_2, B, P; \rho, \varphi), \\ \frac{1}{\tilde{e}^4 \tilde{m}_r} \hat{E}(\tilde{e}, \tilde{m}_1, \tilde{m}_2, \tilde{B}, \tilde{P}) &= \frac{1}{e^4 m_r} \hat{E}(e, m_1, m_2, B, P). \end{aligned} \quad (23)$$

It is worth mentioning that similar scaling relations can be written for three-dimensional case [12].

B. The effective potential and optimal gauge.

The form of the Schrödinger equation (14) implies the existence of the gauge-invariant effective potential

$$V_{eff} = \frac{(\mathbf{P} - e \mathbf{B} \times \boldsymbol{\rho})^2}{2M} - \frac{e^2}{\rho}$$

which describes the relative motion [19]. In Cartesian coordinates choosing without loss of generality the CM momentum $\mathbf{P} = P \hat{\mathbf{y}}$, we have

$$V_{eff}(x, y) = \frac{P^2}{2M} + \frac{e^2 B^2}{2M}(x^2 + y^2) - \frac{e B P}{M}x - \frac{e^2}{\sqrt{x^2 + y^2}}. \quad (24)$$

For any P the potential V_{eff} has a minimum at $x = y = 0$, it corresponds to the Coulomb singularity. It can be called the Coulomb minimum. For a certain values of P , larger than some critical Pseudomomentum (CMS momentum), P_{saddle} another minimum can occur. It is located along the line perpendicular to the direction of Pseudomomentum. In this direction, at $y = 0$, V_{eff} reads

$$V_{eff}(x, 0) = \frac{P^2}{2M} + \frac{e^2 B^2}{2M}x^2 - \frac{e B P}{M}x - \frac{e^2}{|x|}. \quad (25)$$

and the position x_0 of minimum is given by a solution of the cubic equation

$$x_0^3 - \frac{P}{e B}x_0^2 + \text{sign}[x_0]\frac{M}{B^2} = 0. \quad (26)$$

All three solutions of (26) are real if

$$P \geq P_{saddle} \equiv \left(\frac{27}{4} e^3 B M \right)^{\frac{1}{3}}. \quad (27)$$

At $P = P_{saddle} = (\frac{27}{4} e^3 B M)^{\frac{1}{3}}$ the Eq.(26) has double zero which corresponds to the appearance of the saddle point in (25). It is located at $x_{saddle} = (\frac{2M}{B^2})^{\frac{1}{3}}$ (which is charge independent(!), $e > 0$). For $P > P_{saddle}$, the potential (25) has two minima (see Fig.1). For fixed B in the limit $P \rightarrow \infty$ we can easily obtain from (26) the expression

$$x_{0,min} \approx \frac{P}{e B} - \frac{e^2 M}{P^2} + \dots, \quad (28)$$

therefore, $x_{0,min}$ grows linearly at large P and $V_{eff}(x_{0,min}, 0)$ tends to zero as $-\frac{B e^3}{P}$. Similarly, the position of the maximum of the effective potential $V_{eff}(x, 0)$,

$$x_{0,max} \approx \sqrt{\frac{e M}{P B}} + \frac{e^2 M}{2 P^2} + \dots, \quad (29)$$

thus, $x_{0,max} \rightarrow 0$ with growth of P and $V_{eff}(x_{0,max}, 0) \rightarrow \infty$. The behavior of the barrier height $\Delta V = V_{eff}(x_{0,max}, 0) - V_{eff}(x_{0,min}, 0)$ at large P is given by the expansion

$$\Delta V = \frac{P^2}{2M} - \sqrt{\frac{4B e^3 P}{M}} + \frac{3B e^3}{2P} + \sqrt{\frac{B^3 e^9 M}{16 P^5}} + \dots \quad (30)$$

For $P = 0$ the second minimum in V_{eff} (25) does not exist and the potential possesses azimuthal symmetry. In this case, the symmetric gauge emerges naturally as the most convenient. The convenience is related with the fact that for this gauge the ground state eigenfunction is real. For $P \neq 0$ the azimuthal symmetry is broken, consequently, the most convenient choice of the gauge to treat the problem is no longer evident. A question can be posed: in what gauge the ground state eigenfunction is real? In such a gauge the trial function for the ground state can be searched among real functions. This strategy was realized in [13].

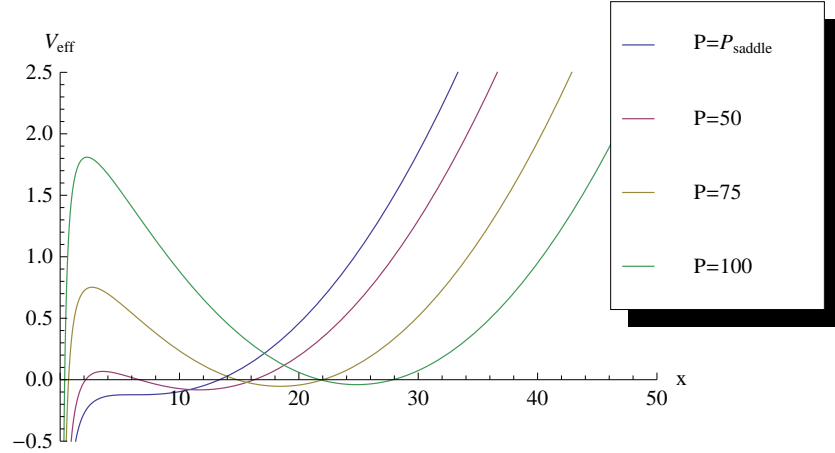


Figure 1: Hydrogen atom: effective potential V_{eff} (25) at $P = P_{saddle}, 50, 75, 100$. $P_{saddle} = 36.7$ and $B = B_0 = 9.3918 \times 10^9 \text{ G}$.

Since we are going to use an approximate method for solving the Schrödinger equation with the Hamiltonian (14), a quality of the approximation of ground state function can depend on the gauge. In particular, one can ask whether can one find a gauge for which a given trial function leads to minimal variational energy. Such a gauge (if found) can be called optimal for a chosen trial function.

To this end, it is convenient to introduce a unitary transformation

$$U = e^{-ie(\mu_2 - \mu_1) \mathbf{A}_{\rho_0} \cdot \boldsymbol{\rho}}, \quad (31)$$

where

$$\boldsymbol{\rho}_0 = \frac{dP}{eB} \hat{\mathbf{x}} \quad (32)$$

and $0 \leq d \leq 1$ is a parameter. The unitary transformed Hamiltonian (14) takes the form

$$h_d \equiv U^{-1} h U = \frac{(\hat{\mathbf{p}} - e(\mu_2 - \mu_1) \mathbf{A}_{(\boldsymbol{\rho} - \boldsymbol{\rho}_0)})^2}{2m_r} + \frac{(\mathbf{P} + e\mathbf{B} \times \boldsymbol{\rho})^2}{2M} - \frac{e^2}{\rho}, \quad (33)$$

This transformation implies that we consider now the Schrödinger equation in a linear gauge for which the position of the gauge center, where $\mathbf{A}(x, y) = 0$, is located at $y = 0$, $x = \frac{dP}{eB}$. For $P > P_{saddle}$ we expect the gauge center to be localized on the line $y = 0$, between the origin $x = 0$ and the second minimum $x = x_{0,min}$ of V_{eff} , (see (28)). Thus, the vector potential can be considered as a variational function and can be chosen by a procedure of minimization as it was proposed in [13] (see also for discussion [14]). The case $d = 0$ has been used in the past to study the so-called centered states with wavefunction peaked at the Coulomb minimum [16]. While for the so-called "decentered" states it seems natural to consider $d = 1$. The eigenvalue problem

$$h_d \chi_{\mathbf{P}} = E \chi_{\mathbf{P}}, \quad (34)$$

where $\chi_{\mathbf{P}} = e^{ie(\mu_2 - \mu_1) \mathbf{A}_{\rho_0} \cdot \boldsymbol{\rho}} \psi_{\mathbf{P}}$, is the central object of our study hereafter.

C. Asymptotics.

If we put $\chi_{\mathbf{P}} = e^{-\varphi}$ in (34), one can construct the WKB-expansion at large $\rho = \sqrt{x^2 + y^2}$ for the phase φ . The leading term at $\rho \rightarrow \infty$ is given by

$$\varphi = \frac{eB}{4} \rho^2 + O(\rho). \quad (35)$$

Assuming the condition (27) is fulfilled, the potential (26) has the second minimum at $x_0 \neq 0$. It can be constructed the double Taylor expansion of the phase at $x = x_0, y = 0$,

$$\varphi = \alpha_0 + \alpha_2 (x - x_0)^2 + \alpha_3 (x - x_0)^3 + \alpha_4 (x - x_0)^4 + \dots + \beta_2 y^2 + \beta_4 y^4 + \dots + \gamma_3 (x - x_0) y^2 + \dots \quad (36)$$

where α_0 is unimportant constant and

$$\alpha_2 = E_x m_r, \quad \alpha_3 = \frac{e^2}{6 E_x x_0^4}, \quad \alpha_4 = \frac{1}{6} m_r \left(2 E_x^2 m_r - \frac{e^2 B^2}{2 M} + \frac{e^2}{x_0^3} \right),$$

$$\beta_2 = E_y m_r, \quad \beta_4 = \frac{1}{6} m_r \left(2 E_y^2 m_r - \frac{e^2 B^2}{2 M} - \frac{e^2}{2 x_0^3} \right), \quad \gamma_3 = -\frac{e^2}{2 E_x x_0^4},$$

here $E = E_x + E_y$. Similarly, at $x = 0, y = 0$,

$$\varphi = 2 m_r \rho + O(\rho^2). \quad (37)$$

D. Approximations

Making interpolation between WKB-expansion (35) and the perturbative expansion (37), (36), respectively, we arrive at the following expressions

$$\varphi_c = \frac{A_0 + A_1 \rho + A_2 x \rho + A_3^2 \rho^3}{\sqrt{1 + A_4 x + A_5^2 \rho^2}} - \frac{\alpha_c}{2} \log(1 + A_4 x + A_5^2 \rho^2) \quad (38)$$

$$\varphi_m = \frac{D_0 + D_1 \tilde{x}^2 + D_2 y^2 + D_3^2 \varrho^4}{\sqrt{1 + D_4 \tilde{x}^2 + D_5 y^2 + D_6^2 \varrho^4}}$$

where $\tilde{x} = x - x_m$, $\varrho^2 = \tilde{x}^2 + y^2$ and $A's$, $D's$, α_c , x_m are non-linear variational parameters. Following the prescription formulated in [11] we construct a trial function for the ground state in a form of linear superposition

$$\chi_{\mathbf{P}} = C_1 e^{-\varphi_c} + C_2 e^{-\varphi_m}, \quad (39)$$

where $C's$ are linear variational parameters. Supposedly, they should behave smoothly as a function of a magnetic field.

IV. RESULTS

We carried out a variational study of the two-body neutral system on a plane moving across a magnetic field. The main emphasis is to explore stability of the moving system, thus, studying the ground state. For the case of Hydrogen atom, the energy for several magnetic fields $0 < B < 1000$ a.u. and values of Pseudomomentum (= CMS momentum P) $0 \leq P < 200$ a.u. is presented in Table II. The energy grows monotonically and rather

sharp as a function of a magnetic field for fixed Pseudomomentum but at much slow pace as a function of Pseudomomentum for a fixed magnetic field. It is worth noting that for fixed B the energy E as a function of P tends asymptotically to the ground state energy of two non-interacting charges in a magnetic field.

After making a minimization, one can see the appearance of a sharp change in behavior of parameters in (39) as a function of P . It is related with a fact of the existence of a certain critical Pseudomomentum $P_c > P_{saddle}$ such that for $P < P_c$ the optimal linear parameters $C_1 \approx 1$, $C_2 \approx 0$ the wavefunction has a peak near the Coulomb singularity (centered state). At $P > P_c$ the situation gets opposite: the parameters $C_1 \approx 0$, $C_2 \approx 1$ and the wavefunction is peaked near the second well of (25), see Fig.1 (we call this well the *magnetic* well) which corresponds to a decentered state. The existence of such a change in the behavior of parameters results also in a specific behavior of energy dependence (see for example Fig.2) and mean interparticle separation vs the Pseudomomentum. From physical point of view at $P = P_c$ the effective depth of the Coulomb well and one of the magnetic well get equal. If $P < P_c$ the effective depth of the Coulomb well is larger (or much larger depending on a magnetic field strength) than one of the magnetic well, the system prefers to stay at the Coulomb well. If $P > P_c$ the effective depth of the Coulomb well is smaller (or much smaller depending on a magnetic field strength) than one of the magnetic well, the system prefers to stay at the magnetic well. For all studied magnetic fields the barrier between wells is very large, the probability of tunneling from one well to another one is very small. Hence, the energy behavior *vs.* CMS momentum is defined by the behavior in one well or another, it is close to classical behavior. Thus, the presence of the second minimum in the effective potential can be neglected. This phenomenon is very well-pronounced at small magnetic fields. Similar behavior was observed in three-dimensional case in [10] (for Hydrogen atom) and [17] (for Positronium). The behavior of P_c as a function of magnetic field is presented in Fig. 3, P_c grows with an increase of B . Typical distribution $|\chi_{\mathbf{p}}|^2$ for $P < P_c$ and $P > P_c$ is shown on Fig. 4.

The evolution of the gauge center parameter d (see (32)) *vs.* CMS momentum is shown in Table III. For $P < P_c$ the parameter d is very small, it varies within $[0 - 0.051]$ for magnetic field range $0.1 - 1000$ a.u. while for $P > P_c$ it is close to 1, it varies within $[0.985 - 1]$ for magnetic field range $0.1 - 10$ a.u. Thus, the gauge changes from the symmetric gauge centered at the Coulomb well to symmetric gauge but centered at the magnetic well. In turn,

the parameter d remains almost equal to 0 up to $P = P_c$ (which means the gauge center coincides with a position of the Coulomb singularity, then sharply jumps to a value close to 1 (gauge center coincides with a position of the minimum of magnetic well), displaying a behavior which looks like a phase transition. But it is not a phase transition: the energy changes sharply but smooth. For $P = P_c$ the parameter $d \sim 0.5$. There exists a certain domain of transition from one regime to another. Overall situation looks very similar to one for the H_2^+ molecular ion in a magnetic field in inclined configuration [13].

In order to illustrate the transition from a centered state to a decentered one we have calculated, using the trial function (38) with optimal parameters, the expectation value of the relative coordinate, $\langle \rho \rangle$, see Table IV. At weak magnetic fields B , the transition is very sharp, becoming even more pronounced with a magnetic field decrease. For all studied magnetic fields and fixed CMS momentum $\langle \rho \rangle$ is finite. Furthermore, the trial function (38) remains normalizable in relative coordinates $\boldsymbol{\rho}$, see (13). It indicates stability of the neutral system.

To complete the study we show in Tables VII - XIII (see Supplementary Materials) the nonlinear parameters A 's, D 's and α_c of the trial function (38) as a function of the magnetic field strength for the optimal configuration. For all considered values of Pseudomomentum the parameter $A_1 = 1.998, 1.998, 1.982, 1.965, 1.938$ at $B = 0.1, 1, 10, 100, 1000$ a.u., respectively. A deviation $|A_1 - 2|$ measures (anti)-screening of the electric charge due to the presence of a magnetic field. The optimal value of energy corresponds to $x_m \approx x_{0,min}$.

Our variational results are checked on agreement with results obtained in other methods. Comparison with perturbative theory in the high-magnetic-field limit (taking the Coulomb interaction as a perturbation) is presented in Table V. Let us note that with the increase of a magnetic field the variational and perturbative results get closer and for $B = 1000$ a.u. they agree in four significant digits. We adopted the Lagrange mesh method based on the Vincke-Baye approach [15] to obtain the ground energy for $B = 1$ a.u. and different Pseudomomenta P , see Table VI. For all studied values of P the variational energy is in agreement with Lagrange mesh calculations in not less than 5 s.d.

It is quite interesting to make a comparison with a single numerical study by Lozovik *et al.* [8] of direct excitons in GaAs/Al_{0.33}Ga_{0.67}As CQW's. This study was done for very small values of magnetic field only. It can be seen that variational energies based on (38) are systematically lower in $\sim 10\%$. Qualitative behavior of variational energy as a function of

Pseudomomentum P is similar to one presented in [8], see Fig. 5.

P	E				
	$B = 0.1$	$B = 1$	$B = 10$	$B = 100$	$B = 1000$
0	-1.9914	-1.4587	11.299	174.124	1918.98
1	-1.9912	-1.4585	11.299	174.124	1918.98
25	-1.8213	-1.2887	11.468	174.291	1919.15
50	-1.3110	-0.7787	11.976	174.794	1919.63
75	-0.4604	0.0713	12.823	175.631	1920.44
100	0.19589 ^d	1.261	14.009	176.803	1921.57
125	0.19669 ^d	1.966 ^d	15.534	178.310	1923.02
150	0.19722 ^d	1.972 ^d	17.398	180.152	1924.80
175	0.19760 ^d	1.976 ^d	19.600	182.329	1926.90
200	0.19789 ^d	1.978 ^d	19.788 ^d	184.840	1929.32

Table II: Ground state energy E in Hartrees (see (34)); magnetic field B and Pseudomomentum P in effective atomic units, $B_0 = 9.3917 \times 10^9$ G , $P_0/\hbar = 3.47 \times 10^{11}$ cm⁻¹, respectively. Energies corresponding to decentered states marked by ^d (see text).

V. CONCLUSIONS

Summarizing, we want to state that a simple uniform approximation of the ground state eigenfunction for the two-dimensional moving Hydrogen atom and Positronium in a

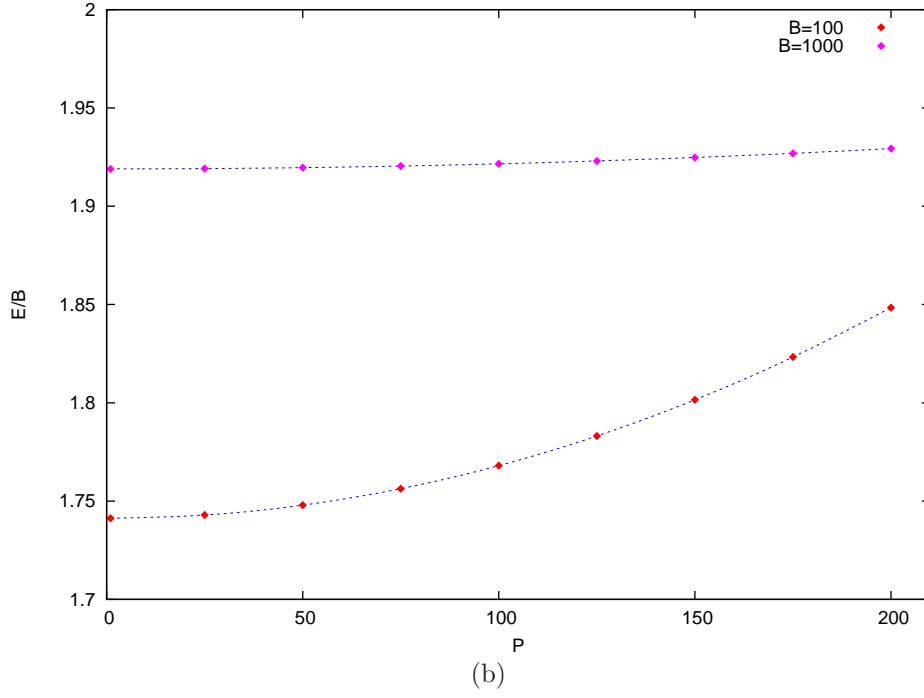
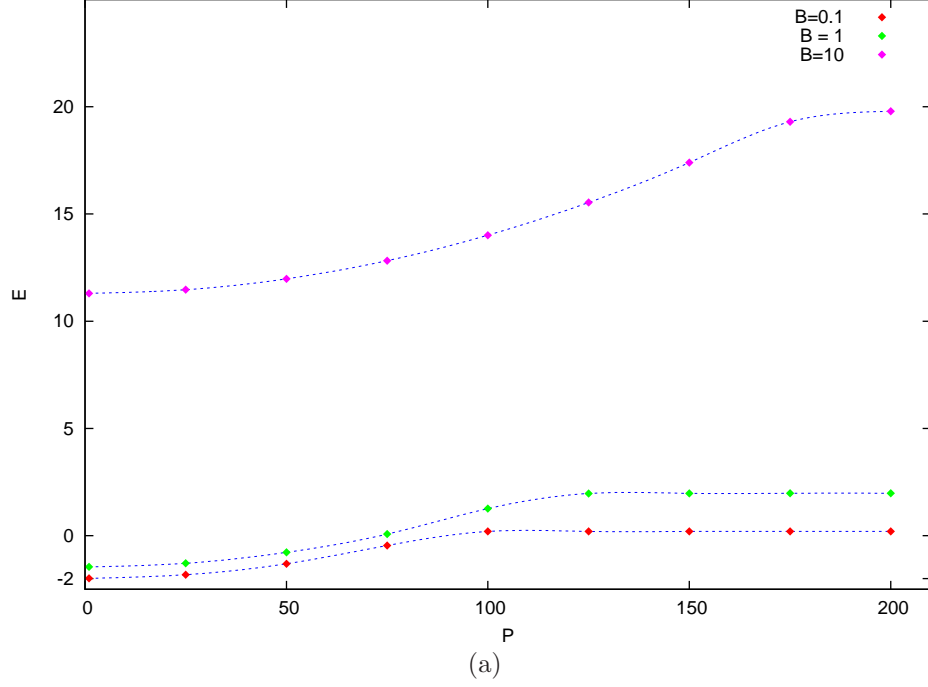


Figure 2: The energy (in Hartrees) of ground state *vs* Pseudomomentum P . (a) E *vs* P for magnetic fields $B = 0.1, 1, 10$. (b) E/B *vs* P for magnetic fields $B = 10^2, 10^3$ a.u.; magnetic field B and Pseudomomentum P in effective atomic units, $B_0 = 9.3917 \times 10^9$ G , $P_0/\hbar = 3.47 \times 10^{11}$ cm $^{-1}$, respectively.

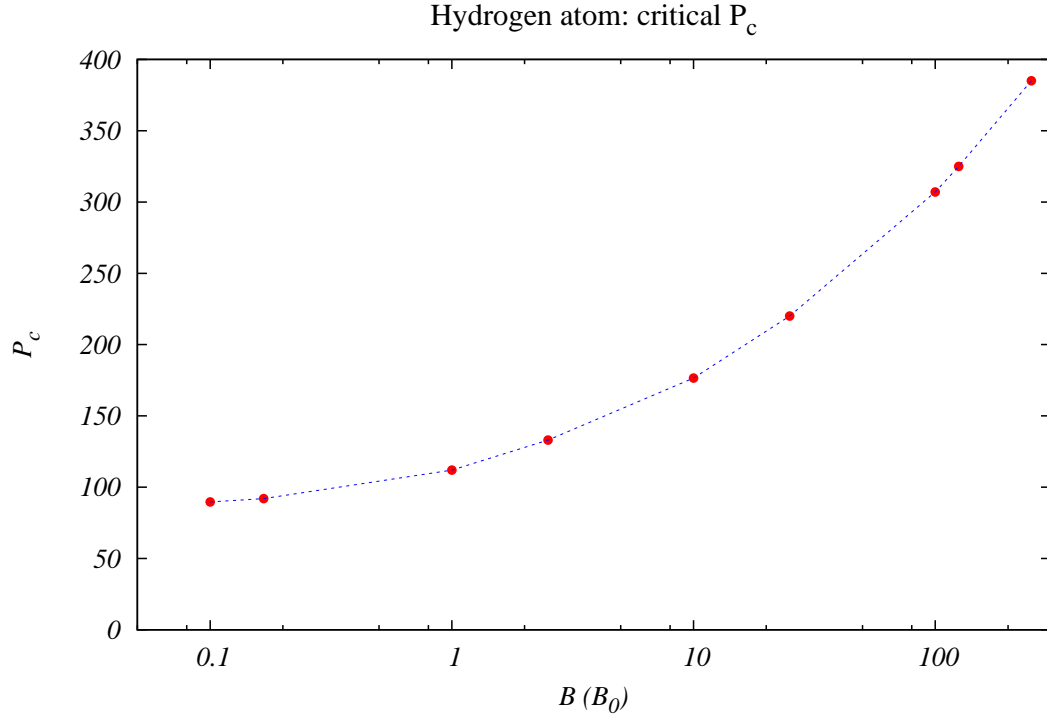


Figure 3: Critical Pseudomomentum P_c vs B .

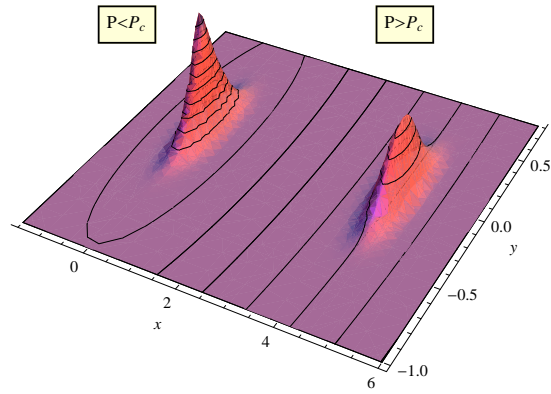


Figure 4: Hydrogen atom: the variational density of the ground state function $|\chi_{\mathbf{P}}|^2$ of Hamiltonian (34) at $P < P_c$ (left peak) and $P > P_c$ (right peak) for $B = 10$ a.u. Magnetic field in effective atomic units, $B_0 = 9.3917 \times 10^9 G$

P	d				
	$B = 0.1$	$B = 1$	$B = 10$	$B = 100$	$B = 1000$
$P < P_c$	0	0.0005	0.004	0.0156	0.051
$P > P_c$	1	1	0.985	—	—

Table III: Optimal gauge parameter d (see (32)) for different magnetic fields and Pseudomomenta; magnetic field in effective atomic units, $B_0 = 9.3917 \times 10^9$ G.

P	$\langle \rho \rangle$		
	$B = 0.1$	$B = 1$	$B = 10$
0	0.49	0.39	0.175
75	0.49	0.39	0.175
100	250^d	0.39	0.175
125	312^d	31^d	0.175
150	375^d	37^d	0.175
175	437^d	43^d	0.175
200	500^d	50^d	4.9^d

Table IV: Expectation value $\langle \rho \rangle$: magnetic field in effective atomic units, $B_0 = 9.3917 \times 10^9$ G. At $B = 100, 1000$ a.u., $\langle \rho \rangle \approx 0.06, 0.019$, respectively. Data corresponding to decentered states marked by d (see text). For $P < P_c$, $\langle \rho \rangle \approx 0$, while for $P > P_c$, $\langle \rho \rangle \approx \langle x \rangle \approx x_{0,min} \propto P$.

magnetic field is constructed. It manifests an approximate solution of the problem. The key element of the procedure is to make an interpolation between the WKB expansion at large distances and perturbation series at small distances both for the phase of the wavefunction; in other words, to find an approximate solution for the corresponding eikonal equation. In general, the separation of variables helps us to solve this problem easily. In our case of non-separability of variables the WKB expansion of a solution of the eikonal equation cannot be constructed in a unified way, since it depends on the way to approach to infinity. However, a reasonable approximation of the first dominant growing terms of the WKB expansion of

B	E	
	E_0	E_0^L
0.1	-1.9914	-0.592
1	-1.4587	-0.506
10	11.299	12.066
100	174.124	174.83
1000	1918.98	1919.68

Table V: Ground state energy in Hartrees. E_0 from (38) and E_0^L from perturbation theory. Magnetic field in effective atomic units, $B_0 = 9.3917 \times 10^9$ G.

P	E	
	E_0	E_0^{mesh}
0	-1.45879	-1.45879
1	-1.45852	-1.45852
25	-1.28877	-1.28877
50	-0.77872	-0.77871
75	0.07136	0.07137
100	1.26149	1.26149

Table VI: Ground state energy at $B = B_0$. E_0 from (38) and E_0^{mesh} obtained with the Lagrange mesh method (parameter d taken from the corresponding variational results based on (38)). Magnetic field in effective atomic units, $B_0 = 9.3917 \times 10^9$ G.

the phase of wavefunction seems sufficient to construct the interpolation between large and small distances giving the results of rather high accuracy.

It was demonstrated that for all magnetic fields and all CMS momenta a neutral system which moves across a magnetic field along the plane is bound. Its energy grows with a magnetic field strength increase as well as CMS momentum increase. For fixed magnetic field B energy behavior demonstrates a sharp change for a certain value of CMS momentum

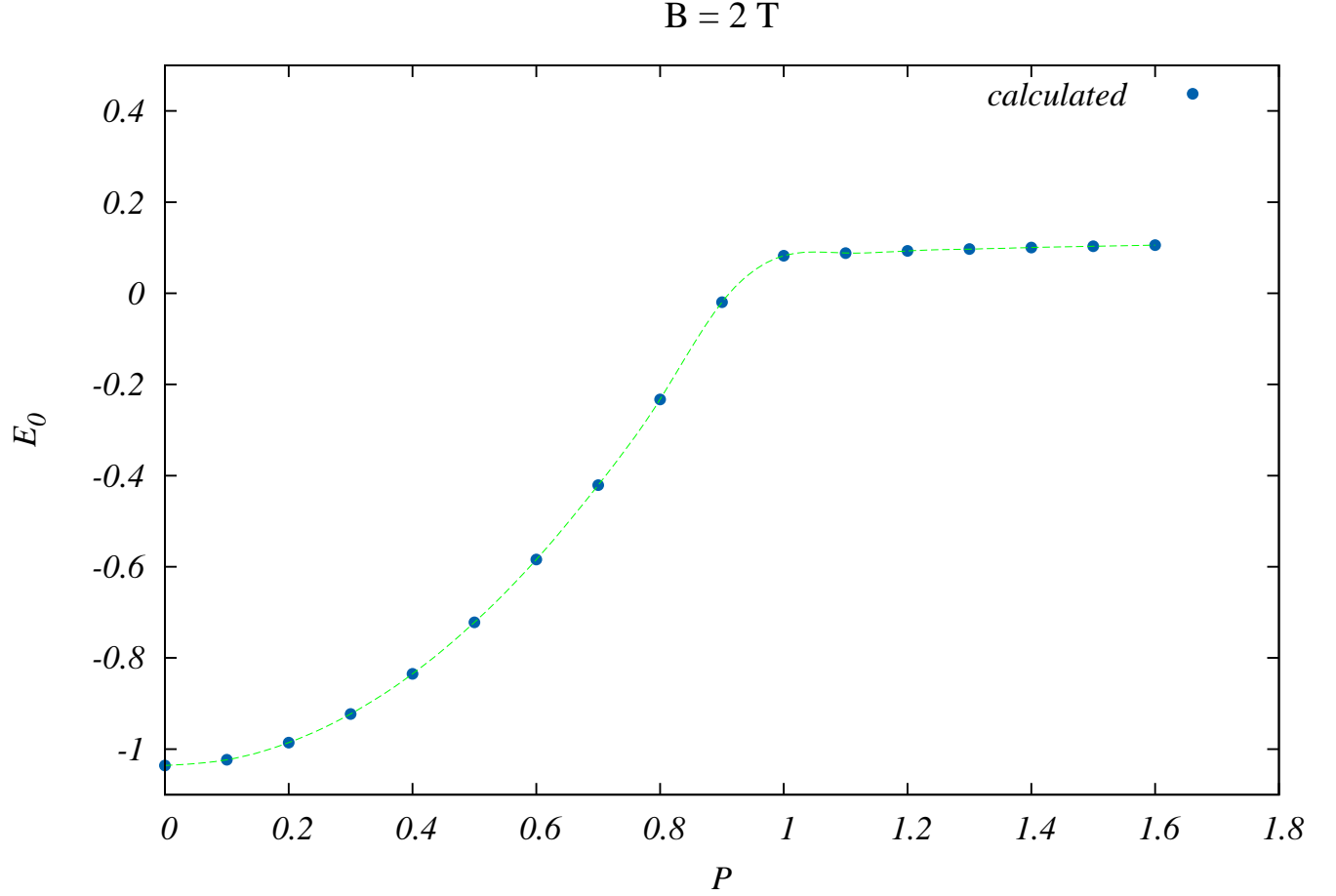


Figure 5: Ground state energy: Direct excitons in GaAs/Al_{0.33}Ga_{0.67}As CQWs with $\epsilon = 12.1$ at $B = 2 \text{ T}$ studied in [8], see Fig.5. Present results are marked by bullets. The units used are the same as in [8].

$P_c(B)$. It seems this phenomenon can be used to measure a magnetic field strength. This effect was already mentioned in the case of three-dimensional Hydrogen atom moving across magnetic field [18].

We calculated the corrections to the energy and to the wavefunction for the ground state of the Hydrogen atom and Positronium in a double perturbation theory in B and P since the ground state remains nodeless. This became possible as a result of the application of the *nonlinearization* method, since it is difficult to perform such calculations within the framework of the standard approach with use of sums over intermediate states or Green functions. In particular, we succeeded in computing the crossterms $\sim B^n P^k$ for arbitrary

masses m_1, m_2 . It is quite non-trivial task due to non-separability of variables in original Hamiltonian. To the authors knowledge, the corrections to the energy and to the wave function of orders $B^2 P^2$, and $B^4 P^2$ (cross terms) are reported for the first time. Concrete results for the Hydrogen atom and Positronium are presented in Table I. In general, the correction $\Phi_{n,k}$ to the phase of wave function for even k is non-vanishing, while for odd k it is pure imaginary(!), except for the case of equal masses, e.g. Positronium. Since the procedure exploited was purely algebraic, one can use symbolic calculation routines like MAPLE to find higher order corrections analytically. However, it should be kept in mind that perturbation theory in B and P series is divergent.

Acknowledgments

The authors are grateful to J. C. López Vieyra and H. Olivares Pilon for their interest in the present work, helpful discussions and important assistance with computer calculations. This work was supported in part by the University Program FENOMECE, and by the PAPIIT grant **IN109512** and CONACyT grant **166189** (Mexico).

-
- [1] M.A. Escobar-Ruiz and A.V. Turbiner,
Two charges on a plane in a magnetic field: special trajectories
Journal of Math Physics **54**, 022901 (2013)
 - [2] A.V. Turbiner and M.A. Escobar-Ruiz,
Two charges on a plane in a magnetic field: hidden algebra, (particular) integrability, polynomial eigenfunctions,
J. Phys. A: **46** , 295204 (2013)
 - [3] M. Taut,
Two electrons in a homogeneous magnetic field: particular analytical solutions,
J. Phys. **A27**, 1045 (1994)
 - [4] M. Taut,
Two particles with opposite charge in a homogeneous magnetic field: particular analytical solutions of the two-dimensional Schrödinger equation,
J. Phys. **A32** (1999) 5509 - 5515
 - [5] A.V. Turbiner,
Two electrons in an external oscillator potential: The hidden algebraic structure
Phys. Rev. A **50**, 5335 (1994)
 - [6] M.A. Escobar-Ruiz and A.V. Turbiner,
Two charges on plane in a magnetic field I. “Quasi-equal” charges and neutral quantum system at rest cases
Annals of Physics **340** (2014) 37-59
 - [7] L.P. Gorkov, I.E. Dzyaloshinskii,
Contribution to the Theory of the Mott Exciton in a Strong Magnetic Field,
ZhETF **53** (1967) 717-722;
Sov. Phys. JETP **26** (1968) 449-451 (English translation)
 - [8] Yu.E. Lozovik, I.V. Ovchinnikov, S.Yu. Volkov, L.V. Butov, and D.S. Chemla,
Quasi-two-dimensional excitons in finite magnetic fields,
Phys. Rev. B **65**, 235304 (2002)

- [9] A.V. Turbiner,
*A New Approach to Finding Levels of Energy of Bound States
in Quantum Mechanics: Convergent Perturbation Theory,*
Soviet Phys. – Pisma ZhETF **30**, 379-383 (1979).
JETP Lett. **30**, 352-355 (1979) (English Translation);
*The Problem of Spectra in Quantum Mechanics and the ‘Non-Linearization’
Procedure,*
Soviet Phys. – Usp. Fiz. Nauk. **144**, 35-78 (1984),
Sov. Phys. Uspekhi **27**, 668-694 (1984) (English Translation)
- [10] P. Schmelcher and L.S. Cederbaum,
*Intermittent chaos in Hamiltonian systems: The three-dimensional hydrogen atom in magnetic
fields* *Phys. Rev. A* **47** 2634 (1993)
- [11] A.V. Turbiner,
Multi-Dimensional Anisotropic Anharmonic Oscillator (Quantitative Approach),
Soviet Scientific Reviews **10**, 79-131 (1988) (Gordon & Breach Publishers);
Anharmonic oscillator and double-well potential: approximating eigenfunctions,
Letters in Mathematical Physics **74**, 169-180 (2005);
Double well potential: perturbation theory, tunneling, WKB (beyond instantons),
Intern.Journ.Mod.Phys. **A25**, 647-658 (2010)
- [12] H. Herold, H. Ruder and G. Wunner,
J. Phys. B **14**, 751 (1981)
- [13] A.V. Turbiner and J.C. López Vieyra, *One-electron Molecular Systems in a Strong Magnetic
Field,* *Phys. Repts.* **424**, 309-396 (2006)
- [14] M. Vincke, M. Le Dourneuf and D. Baye,
*Hydrogen atom in crossed electric and magnetic fields: transition from weak to strong electron-
electron decentring,*
J. Phys. B: At. Mol. Opt. Phys. **25** (1992) 2787 - 2807
- [15] M. Vincke and D. Baye,
Hydrogen molecular ion in an aligned strong magnetic field by the Lagrange-mesh method,
J. Phys. B: At. Mol. Opt. Phys. **39** (2006) 2605 - 18
- [16] L.A. Burkova, I.E. Dzyaloshinskii, G.F. Drukarev, and B.S. Monozon,

- Hydrogen-like system in crossed electric and magnetic fields,*
Sov. Phys. JETP **44**, 276 (1976)
- [17] J.Ackermann, J.Shertzer and P.Schmelcher,
Phys.Rev.Lett. **78**, 199 (1997)
- [18] A.Y Potekhin,
Structure and radiative transitions of the hydrogen atom moving in a strong magnetic field,
J. Phys. B: At. Mol. Opt. Phys. **27** (1994) 1073 ;
Hydrogen atom moving across a strong magnetic field: analytical approximations,
J. Phys. B: At. Mol. Opt. Phys. **31** (1998) 49
- [19] It is worth mentioning that in three-dimensional case after pseudoseparation of variables the Schrödinger equation describing the relative motion is also characterized by gauge-invariant effective potential [10]

Hydrogen atom: critical P_c

